

## **Implementation of Dynamic Data Evaluation for Pure Compounds: Problems and Algorithms**

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Traditional critical data evaluation is an extremely time and resource consuming process, which includes extensive manpower applied to data collection, mining, analysis, fitting, etc. Furthermore, it must be performed far in advance of need, which has led to a significant part of the existing recommended data having never been used. The concept of “dynamic” data evaluation was developed by TRC at NIST, and requires large electronic databases (such as the TRC Source data system) capable of storing essentially all of the ‘raw/observed’ experimental data known to date with descriptions of relevant metadata and defined uncertainties. In combination with expert-system software this system allows production of recommended property values (with uncertainties) dynamically or ‘to order.’ Aspects of the implementation of Dynamic Data Evaluation will be discussed including thermodynamic consistency between related properties, selection of fitting equations, use of estimated properties, and uncertainty propagation. The output of the software being designed includes complete sets of thermodynamic property data with reliable uncertainties for any (including hypothetical) organic compound.